

Spin-orbit coupling and g -factor of X -valley in cubic GaN

K. Shen,¹ J. Y. Fu,² and M. W. Wu^{1,*}

¹*Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China*

²*Department of Physics, Qufu Normal University, Qufu, Shandong, 273165, China*

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We report our theoretical investigation on the spin-orbit coupling and g -factor of the X -valley in cubic GaN. We find that the spin-orbit coupling coefficient from $sp^3d^5s^*$ tight-binding model is $0.029\text{ eV}\cdot\text{\AA}$, which is comparable with that in cubic GaAs. By employing the $\mathbf{k}\cdot\mathbf{p}$ theory, we find that the g -factor in this case is only slightly different from the free electron g -factor. These results are expected to be important for the on-going study on spin dynamics far away from equilibrium in cubic GaN.

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Due to the existence of the wide energy gap between the conduction band and the valence band, GaN has been proposed to be a promising candidate for many electronic applications, such as the solid-state ultraviolet optical sources and high-power electronic devices.¹ Recently, the discovery of the room-temperature ferromagnetism in GaN based materials^{2,3} highlights its possible application in future spintronic devices.⁴⁻⁷ Another outstanding property of GaN for realizing the spintronic devices is the extremely long spin lifetime,⁸ because of the relatively weak spin-orbit coupling (SOC) compared to the narrow-gap III-V compounds, such as GaAs and InAs.^{9,10}

For a detailed understanding of the spin dynamics, the SOC is essential.⁷ In cubic GaN, the inequality of the cation and anion in the crystal leads to the bulk inversion asymmetry, which results in the Dresselhaus SOC.¹¹ Up to date, the investigation on spin properties in GaN is focused on the low energy case, where only the lowest valley, i.e., Γ -valley is relevant. Recently, Fu and Wu reported the Dresselhaus SOC coefficient of the Γ -valley, $0.51\text{ eV}\cdot\text{\AA}^3$, from the sp^3s^* tight-binding (TB) model.¹² This result agrees with the later experiment by the time-resolved Kerr rotation measurement.¹³ However, for the spin dynamics under the influence of high electric field¹⁴ or with spin pumping by high-energy laser,¹⁵ electrons can be driven into the high valleys.¹⁴ This multivalley correlation was proposed to be able to induce the charge Gunn¹⁶ and spin Gunn¹⁷ effects in GaAs. Zhang *et al.*¹⁸ investigated the spin dynamics under the high electric field in GaAs quantum wells and suggested that the spin Gunn effect can be hindered by the fast spin relaxation of upper valley (L -valley) and hot-electron effect. To our best knowledge, there has been no report on the multivalley spin dynamics in GaN till now. Since the upper valley in GaN is the X -valley (no L -valley exists in cubic GaN), one may expect different multivalley spin properties in this material. Therefore, the details of the SOC in GaN is required. In our previous work, the expression of the SOC of the X -valley in cubic III-V semiconductors was derived,¹⁹ but the corresponding coefficient of GaN is still unavailable. In the present communication, we

calculate this coefficient for further investigations on the spin dynamics in this material. Moreover, the g -factor is also required to take into account the effect of the external magnetic field. Therefore, we will also calculate the g -factor of the X -valley in GaN from the $\mathbf{k}\cdot\mathbf{p}$ theory.

In order to obtain the splitting energy of SOC, one needs to calculate the band structure. One of the most widely used approaches for band structure calculation is the TB theory.²⁰ From our previous work on GaAs, we find that the d -orbitals are important for the spin splitting of the high valleys.^{19,21} Therefore, we employ the $sp^3d^5s^*$ nearest-neighbor TB model with the SOC here.²² The parameters are taken from the work by Jancu *et al.*²³

The spin-orbit splitting of the conduction band around the X -valley is plotted as a function of the momentum along $X \rightarrow K$ and $X \rightarrow W$ directions in Fig. 1(a). One finds that the splitting increases linearly with the momentum in the small momentum regime with respect to the bottom of the X -valley. In the large momentum regime, this monotonic tendency can be violated.

For the states close to the X -point, the splitting can be described by the effective SOC Hamiltonian, $\mathbf{\Omega}(\mathbf{k}) \cdot \boldsymbol{\sigma}$, with $\mathbf{\Omega}$ and $\boldsymbol{\sigma}$ denoting the corresponding effective magnetic field of the conduction band and the Pauli matrices.^{19,24} For the valleys lie in the $[001]$ -direction, one obtains¹⁹

$$\mathbf{\Omega}(\mathbf{k}) = \beta(k_x, -k_y, 0). \quad (1)$$

Here \mathbf{k} represents the momentum measured from the bottom of the valley. Obviously, this term results in the spin-orbit splitting linearly depending on the momentum, i.e., $\Delta E = 2\beta k_{\parallel}$ with $k_{\parallel} = \sqrt{k_x^2 + k_y^2}$ being the magnitude of the transverse momentum.

The SOC coefficient can be measured by $\beta(\mathbf{k}) = \Delta E/(2k_{\parallel})$. The value of β is shown as a function of momentum along $X \rightarrow K$ direction in Fig. 1(b). One can see that in the range of small momentum, β keeps a constant value $0.029\text{ eV}\cdot\text{\AA}$. However, when the momentum lies far away from the bottom of the X -valley, β decreases. In the $X \rightarrow W$ direction, β increases with increasing mo-

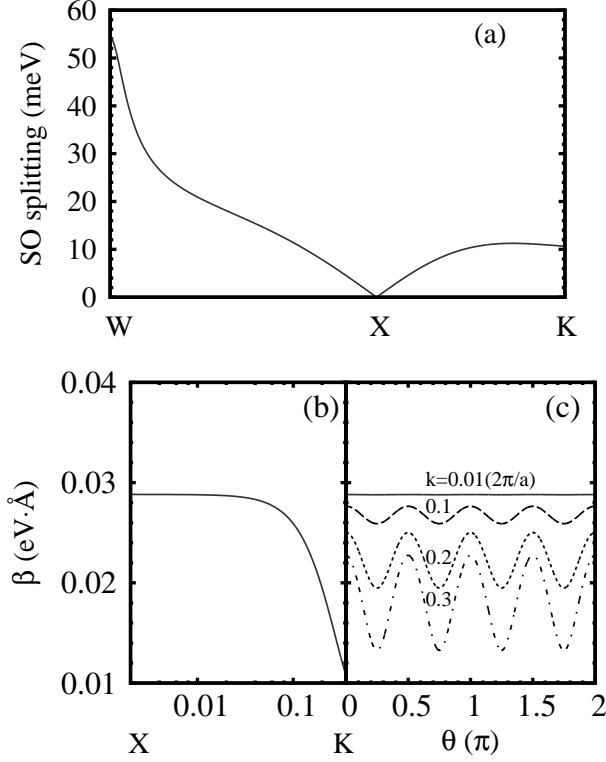


FIG. 1: (a) Spin-orbit splitting of cubic GaN around the X -valley along $X \rightarrow K$ and $X \rightarrow W$ directions. (b) The corresponding SOC parameter β vs. momentum along $X \rightarrow K$ direction. (c) β vs. angle for the momentum lying in the x - y plane. Solid curve: $k=0.01$; dashed curve: 0.1; dotted curve: 0.2; and chain curve: 0.3 ($2\pi/a$), with $a = 4.5$ Å, the lattice constant of cubic GaN.²⁸

mentum (not shown) as expected from Fig. 1(a). This phenomenon is due to the higher order corrections of the SOC terms. We now turn to the effect of the direction of the transverse momentum on the SOC coefficient. In Fig. 1(c), we show the anisotropic behavior of SOC coefficient, where the momentum lies in the x - y plane with θ being the angle between the momentum and x -axis. One can see the angle dependence becomes remarkable for large momentum, which is also from the higher order correction of the SOC. Interestingly, one notices that the SOC coefficient of X -valley obtained here is comparable with that of GaAs, $0.059 \text{ eV}\cdot\text{\AA}$,¹⁹ which is very different from the situation of Γ -valley. For the Γ -valley, the Dresselhaus SOC coefficient in GaN is much smaller than that in GaAs.

We should point out that the d -orbitals are of critical importance in determining the SOC coefficient of the X -valley in GaN. Specifically, we obtain $\beta = 0.002 \text{ eV}\cdot\text{\AA}$ from sp^3s^* TB model parameterized by O'Reilly *et al.*,²⁵ which is one order of magnitude smaller than that from $sp^3d^5s^*$ TB model. As a comparison, we also calculate the SOC coefficient of the Γ -valley from $sp^3d^5s^*$ TB model and obtain $\gamma = 0.235 \text{ eV}\cdot\text{\AA}^3$, which is close to that

from sp^3s^* model $\gamma = 0.508 \text{ eV}\cdot\text{\AA}^3$ (Ref. 12).

Now, we turn to figure out the g -factor of the X -valley based on the $\mathbf{k} \cdot \mathbf{p}$ approach by following the approach given in Ref. 26. In our calculation, we first include the conduction band (X_{1c}) and the valence bands (X_{3v} and X_{5v}) and neglect the contribution of the other remote bands.

Similar to the L -valley case,²⁶ one can write the longitudinal effective mass m_l and the transverse one m_t as²⁶

$$\frac{m_0}{m_l} - 1 = \frac{2}{m_0} \frac{|\langle X_{1c} | p_z | X_{3v} \rangle|^2}{E_{X_{1c}} - E_{X_{3v}}}, \quad (2)$$

and

$$\frac{m_0}{m_t} - 1 = \frac{2}{m_0} \frac{|\langle X_{1c} | p_x | X_{5v} \rangle|^2}{E_{X_{1c}} - E_{X_{5v}}}, \quad (3)$$

respectively.

The longitudinal and transverse g -factors are given by^{26,27}

$$\begin{aligned} g_{\parallel} - g_0 &= -\frac{2}{m_0} \frac{\delta \langle X_{1c} | p_x | X_{5v} \rangle \langle X_{5v} | p_y | X_{1c} \rangle}{(E_{X_{1c}} - E_{X_{3v}})(E_{X_{1c}} - E_{X_{5v}})} \\ &= -\delta \left(\frac{m_0}{m_t} - 1 \right) / (E_{X_{1c}} - E_{X_{3v}}), \end{aligned} \quad (4)$$

and

$$\begin{aligned} g_{\perp} - g_0 &= -\frac{2}{m_0} \frac{\delta' \langle X_{1c} | p_y | X_{5v} \rangle \langle X_{3v} | p_z | X_{1c} \rangle}{(E_{X_{1c}} - E_{X_{3v}})(E_{X_{1c}} - E_{X_{5v}})} \\ &= -\delta' \left[\frac{(m_0/m_t - 1)(m_0/m_l - 1)}{(E_{X_{1c}} - E_{X_{3v}})(E_{X_{1c}} - E_{X_{5v}})} \right]^{1/2} \end{aligned} \quad (5)$$

where $\delta = 2i \langle X_{5v} | h_z | X_{5v} \rangle$ and $\delta' = 2i \langle X_{5v} | h_x | X_{3v} \rangle$ are the matrix elements of the SOC.²⁷ \mathbf{p} describes the momentum operator. g_0 is the g -factor of the free electron.

From our TB calculation, we obtain the energy levels of the X -valley, i.e., $E_{X_{1c}} = 4.58 \text{ eV}$, $E_{X_{5v}} = -2.74 \text{ eV}$, and $E_{X_{3v}} = -6.98 \text{ eV}$. We estimate the matrix element of the SOC from the band splittings of the X_{5v} band and take $\delta' = \delta = 0.02 \text{ eV}$. With $m_l = 0.5m_0$ and $m_t = 0.3m_0$ (Ref. 28), we obtain $g_{\parallel} = 1.996$ and $g_{\perp} = 1.997$ by taking $g_0 = 2$. We should point out that such a small difference of the g -factor in X -valley from g_0 is consistent with the previous results in silicon²⁷ and other III-V group compounds.²⁹

Finally, we would like to discuss the contribution of the remote bands. One may notice that the second conduction band (X_{3c} with $E_{X_{3c}} = 8.21 \text{ eV}$) lies close to the X_{1c} band.³⁰ Since its symmetry is the same as that of the X_{3v} band, it can also contribute to m_l and g_{\perp} . Similar to Eq. (2), one calculates the correction of the longitudinal effective mass due to the X_{3c} band and finds that the condition $\langle X_{1c} | p_z | X_{3c} \rangle / \langle X_{1c} | p_z | X_{3v} \rangle < \sqrt{(E_{X_{3c}} - E_{X_{1c}}) / (E_{X_{1c}} - E_{X_{3v}})} \approx 0.56$ to guarantee the real condition $m_l < m_0$. As a rough estimation, we take $\langle X_{1c} | p_z | X_{3c} \rangle = 0.5 \langle X_{1c} | p_z | X_{3v} \rangle$ and $\langle X_{5v} | h_x | X_{3c} \rangle = \langle X_{5v} | h_x | X_{3v} \rangle$. Then, it is easy to calculate the final perpendicular g -factor $g'_{\perp} = g_0 + (g_{\perp} - g_0)(1 -$

$0.5\eta)/\sqrt{1-0.25\eta}$ with $\eta = (E_{X_{1c}} - E_{X_{3v}})/(E_{X_{3c}} - E_{X_{1c}}) = 3.18$ and g_{\perp} given by Eq. (5). One obtains $g'_{\perp} = 2.004$, which indicates that the relation $g'_{\perp} \approx g_0$ is still preserving by considering the correction from the X_{3c} band.

In summary, we have studied the SOC and g -factor of the X -valley in cubic GaN. By taking into account the possible effect of the d -orbitals on high valleys, we perform our calculation with an $sp^3d^5s^*$ nearest-neighbor TB model. The spin splitting of the conduction band in the X -valley and the corresponding SOC coefficient are

calculated. We find that the SOC coefficient of the X -valley in GaN is $0.029\text{eV}\cdot\text{\AA}$, which is comparable with that in GaAs. In addition, we calculate the g -factor and find that the value is very close to that of the free electron. These results are useful for understanding the spin dynamics far away from the equilibrium.

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* Author to whom correspondence should be addressed; Electronic address: mwwu@ustc.edu.cn.

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